Two-dimensional FT-NIR correlation study of hydrogen bonding in the butan-1-ol/ water system.

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Streszczenie

The effects of temperature and concentration on hydrogen bonding in butan-1-ol/water binary mixtures havebeen studied by using generalized 2D Fourier transform (FT) near-infrared (NIR) correlation spectroscopy.Particular attention has been paid to the analysis of changes in the self-association of butan-1-ol resultingfrom the presence of water. The obtained results indicate that the self-association of butan-1-ol is not influencedby small additions of water. When the molar fraction of water (XH2O) increases, bands due to water appear inthe spectra. The number of correlation peaks suggests the presence of two different species of hydrogen-bonded water. In addition, molecules of non-hydrogen-bonded water dispersed among molecules of butan-1-ol were detected. An increase inXH2Oat constant temperature reduces the population of the polymericspecies of butan-1-ol and leads to growth in the number of free OH groups. WhenXH2Oincreases further, thefree OH groups of butan-1-ol interact with molecules of water. The asynchronous peak originating from therotational isomerism of butan-1-ol disappears from the spectra of the mixtures with higher values ofXH2O.This observation indicates that the molecules of water do not reveal conformational selectivity upon theformation of hydrogen bonds with molecules of butan-1-ol. In contrast, due to larger molecular size, thisselectivity appears for butan-1-ol. Both the temperature- and concentration-dependent correlation spectra provideevidence that in the studied system water-water and alcohol-alcohol interactions dominate, whereas thewater-alcohol interactions are weaker.